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**What is claimed is:**

1. A method for reducing computation time of an analysis of diffraction of incident electromagnetic radiation from a periodic grating having a direction of periodicity, said analysis involving a division of said periodic grating into layers, with an initial layer corresponding to a space above said periodic grating, a final layer corresponding to a substrate below said periodic grating, and said periodic features of said periodic grating lying in intermediate layers between said initial layer and said final layer, a cross-section of said periodic features being discretized into a plurality of stacked rectangular sections, within each of said layers a permittivity and electromagnetic fields being formulated as a sum of harmonic components along said direction of periodicity, application of 10 Maxwell's equations providing an intra-layer matrix equation in each of said intermediate layers equating a product of a wave-vector matrix and first harmonic amplitudes of one of said electromagnetic fields to a second partial derivative of said first harmonic amplitudes of said one of said electromagnetic fields with respect to a direction perpendicular to a 15 plane of said periodic grating, said wave-vector matrix being dependent on intra-layer parameters and incident-radiation parameters, a homogeneous solution of said intra-layer matrix equation being an expansion of said first harmonic amplitudes of said one of said electromagnetic fields into first exponential functions dependent on eigenvectors and eigenvalues of said wave-vector matrix, comprising the steps of:  
20 determination of a layer-property parameter region and a layer-property parameter-region sampling;

determination of a maximum harmonic order for said harmonic components of said electromagnetic fields;

calculation of required permittivity harmonics for each layer-property value in said layer-property parameter region determined by said layer-property parameter-

5 region sampling;

determination of an incident-radiation parameter region and an incident-radiation parameter-region sampling;

calculation of said wave-vector matrix based on said required permittivity harmonics for said each layer-property value in said layer-property parameter region determined by said layer-property parameter-region sampling and for each incident-radiation value in said incident-radiation parameter region determined by said incident-radiation parameter-region sampling;

calculation of eigenvectors and eigenvalues of each of said wave-vector matrices for said each layer-property value in said layer-property parameter region determined by said layer-property parameter-region sampling and for said each incident-radiation value in said incident-radiation parameter region determined by said incident-radiation parameter-region sampling;

caching of said eigenvectors and said eigenvalues of said each of said wave-vector matrices in a memory; and

20 use of said eigenvectors and said eigenvalues for said analysis of said diffraction of said incident electromagnetic radiation from said periodic grating.

2. The method of claim 1 further comprising the step of caching in, said memory, said wave-vector matrices for said each layer-property value in said layer-property parameter region determined by said layer-property parameter-region sampling and for said each incident-radiation value in said incident-radiation parameter region determined by said incident-radiation parameter-region sampling.

3. The method of claim 2 further comprising the step of caching in, said memory, said required permittivity harmonics for said each layer-property value in said layer-property parameter region determined by said layer-property parameter-region sampling.

4. The method of claim 1 further comprising the step of calculating a product of a square root of each of said eigenvalues and a corresponding one of said eigenvectors for said each layer-property value in said layer-property parameter region determined by said layer-property parameter-region sampling and for said each incident-radiation value in said incident-radiation parameter region determined by said incident-radiation parameter-region sampling.

5. The method of claim 4 further comprising the step of caching in said memory, said product of said square root of said each of said eigenvalues and said corresponding one of said eigenvectors for said each layer-property value in said layer-property parameter region determined by said layer-property parameter-region sampling and for said each incident-radiation value in said incident-radiation parameter region determined by said incident-radiation parameter-region sampling.

6. The method of claim 1 wherein another of said electromagnetic fields is expressible as an expansion of second harmonic amplitudes into second exponential

functions dependent on said eigenvectors and said eigenvalues of said wave-vector matrix, application of boundary conditions of said electromagnetic fields at boundaries between said layers provides a boundary-matched system matrix equation, and solution of said boundary-matched system matrix equation provides said diffraction of said 5 incident electromagnetic radiation from said periodic grating, and wherein said use of said eigenvectors and said eigenvalues for said analysis of said diffraction of said incident electromagnetic radiation from said periodic grating comprises the step of:

discretization of a cross-section of a ridge of said periodic grating into a stacked set of rectangles on said substrate;

10 retrieval, from said memory, for each of said rectangles, of said eigenvectors and said eigenvalues of said wave-vector matrix based on said intra-layer parameter values of said each of said rectangles, and based on said incident-radiation parameter values of said incident electromagnetic radiation;

15 construction of said boundary-matched system matrix equation using said eigenvectors and said eigenvalues of said wave-vector matrices retrieved from said memory for said each of said rectangles; and

solution of said boundary-matched system matrix equation to provide said diffraction of said incident electromagnetic radiation from said periodic grating.

7. The method of claim 1 wherein said intra-layer parameters for one of said layers 20 include an index of refraction of a material of said periodic features in said one of said layers, an index of refraction of said initial layer, a length of periodicity of said periodic features, a width of said periodic features in said one of said layers, and an offset distance

of said periodic features in said one of said layers, and said incident-radiation parameters include an angle of incidence of said electromagnetic radiation and a wavelength of said electromagnetic radiation.

8. The method of claim 1 wherein within said each of said layers, any line directed  
5 normal to said periodic grating passes through a single material.

9. The method of claim 1 wherein said initial layer and said final layer are  
mathematically approximated as semi-infinite.

10. The method of claim 1 wherein said layer-property parameter region and said  
incident-radiation parameter region describe a hyper-rectangle.

10 11. The method of claim 1 wherein coefficients of said expansion of said harmonic  
amplitudes of said electromagnetic field into said exponential functions include factors  
which are elements of an eigenvector matrix obtained from said wave-vector matrix, and  
exponents of said expansion of said harmonic amplitudes of said electromagnetic field  
include factors which are square roots of eigenvalues of said wave-vector matrix.

15 12. The method of claim 11 wherein said layer-property parameter-region sampling  
is at a uniform density.

13. The method of claim 11 wherein said layer-property parameter-region sampling  
is at a non-uniform density.

14. The method of claim 12 wherein said layer-property parameter-region sampling  
20 is done on a uniform grid.

15. The method of claim 12 wherein said layer-property parameter-region sampling  
is done on a non-uniform grid.

16. The method of claim 11 wherein at least one dimension of said incident-radiation parameter region has a range of a single value.

17. The method of claim 11 wherein at least one dimension of said layer-property parameter region has a range of a single value.

5       18. A method of determining dimensions of a physical profile of a repeating, regularly-spaced series of structures, comprising the steps of:  
          illuminating a test area of said series of said structures with incident radiation having a plurality of wavelengths, said incident radiation traveling along an optical path;  
10       measuring radiation diffracted from said test area at said plurality of wavelengths to obtain a measured diffraction spectrum;  
          determining an intra-layer range and an intra-layer sampling of intra-layer parameters corresponding to layers of profile shapes to be included in a first sub-library;  
15       determining an incident-radiation range and an incident-radiation sampling of incident-radiation parameters corresponding to said optical path of said incident radiation;  
          generating pre-calculated intra-layer-dependent portions of a diffraction calculation for said intra-layer sampling of said intra-layer parameters within said intra-layer range, and said incident-radiation sampling of said incident-radiation parameters within said incident-radiation range;  
20       caching said pre-calculated intra-layer-dependent portions of said

diffraction calculation for said intra-layer sampling of said intra-layer parameters within said intra-layer range, and said incident-radiation sampling of said incident-radiation parameters within said incident-radiation range;

calculating, utilizing said pre-calculated intra-layer-dependent

5 portions of said diffraction calculation, for each of said profile shapes in said first sub-library, a calculated diffraction spectrum according to said diffraction calculation to provide a second sub-library of calculated diffracted spectra;

indexing said first sub-library of said profile shapes with

corresponding spectra from said second sub-library of said calculated diffraction spectra

10 to provide a library of profile-spectra pairs; and

comparing said measured diffraction spectrum with said calculated diffraction spectra in said library of said profile-spectra pairs to find a best-match calculated spectrum which most closely matches said measured diffraction spectrum, whereby one of said profile shapes corresponding to said best-match calculated spectrum is a best match for said physical profile, and said dimensions of said physical profile are determined to be corresponding dimensions of said one of said profile shapes.

19. The method of claim 18 wherein said optical path includes a focusing mechanism.

20. The method of claim 18 wherein said measuring of said diffracted light involves a measurement of intensity of said diffracted light.

21. The method of claim 18 wherein said measuring of said diffracted light involves a measurement of intensity of said diffracted light, and a phase

difference between polarizations of said diffracted light.

22. The method of claim 18 wherein said comparing of said measured diffraction spectrum with said calculated diffraction spectra in said library to determine a best-match calculated spectrum is performed using a 5 least squares computation.

23. The method of claim 22 wherein said least square computation is performed by selecting a number of sample wavelengths, subtracting said measured diffraction spectrum with said calculated diffraction spectra at said sample wavelengths to determine differences at each of said sample 10 wavelengths, and squaring and summing said differences.

24. An apparatus for determining dimensions of a physical profile of a repeating, regularly-spaced series of structures, comprising:

an electromagnetic radiation source for generating electromagnetic radiation having a plurality of wavelengths;

15 a focusing means for directing said electromagnetic radiation along an optical path to illuminate a test area of said series of said structures with incident radiation;

a photometer for measuring diffraction of said incident radiation from said test area at said plurality of wavelengths to obtain a measured 20 diffraction spectrum;

a first memory;

a look-up table;

means for generating a first sub-library of profile shapes;

means for storing said first sub-library of said profile shapes in a first array of said look-up table;

means for generating pre-calculated intra-layer-dependent portions of a diffraction calculation for an intra-layer sampling of 5 intra-layer parameters within an intra-layer range, and an incident-radiation sampling of incident-radiation parameters within an incident-radiation range, and caching said pre-calculated intra-layer-dependent portions of said diffraction calculation in said first memory;

means for calculating, utilizing said pre-calculated intra-layer-dependent portions of said diffraction calculation, for each of said profile shapes in said first sub-library, a calculated diffraction spectrum according to said rigorous coupled-wave calculation to provide a second sub-library of calculated diffraction spectra,

means for storing said second sub-library of said calculated diffraction spectra in a second array of said look-up table at entries corresponding to corresponding ones of said profile shapes in said first sub-library; and

means for comparing said measured diffraction spectrum with said calculated diffraction spectra in said second array of said look-up table to 20 find a best-match calculated spectrum which most closely matches said measured diffraction spectrum, whereby one of said profile shapes corresponding to said best-match calculated spectrum is a best match for said physical profile, and said dimensions of said physical profile are

determined to be corresponding dimensions of said one of said profile shapes.

25. A method of determining dimensions of a physical profile of a repeating, regularly-spaced series of structures, comprising the steps of:

5 illuminating a test area of said series of said structures with incident radiation having a plurality of angles at a single wavelength, said incident radiation traveling along an optical path;

measuring radiation diffracted from said test area at said plurality of angle to obtain a measured diffraction spectrum;

10 determining an intra-layer range and an intra-layer sampling of intra-layer parameters corresponding to layers of profile shapes to be included in a first sub-library;

15 determining an incident-radiation range and an incident-radiation sampling of incident-radiation parameters corresponding to said optical path of said incident radiation;

20 generating pre-calculated intra-layer-dependent portions of a rigorous coupled wave calculation for said intra-layer sampling of said intra-layer parameters within said intra-layer range, and said incident-radiation sampling of said incident-radiation parameters within said incident-radiation range;

caching said pre-calculated intra-layer-dependent portions of said diffraction calculation for said intra-layer sampling of said

intra-layer parameters within said intra-layer range, and said incident-radiation sampling of said incident-radiation parameters within said incident-radiation range;

5 calculating, utilizing said pre-calculated intra-layer-dependent portions of said diffraction calculation, for each of said profile shapes in said first sub-library, a calculated diffraction spectrum according to said diffraction calculation to provide a second sub-library of calculated diffracted spectra;

10 indexing said first sub-library of said profile shapes with corresponding spectra from said second sub-library of said calculated diffraction spectra to provide a library of profile-spectra pairs; and

15 comparing said measured diffraction spectrum with said calculated diffraction spectra in said library of said profile-spectra pairs to find a best-match calculated spectrum which most closely matches said measured diffraction spectrum, whereby one of said profile shapes corresponding to said best-match calculated spectrum is a best match for said physical profile, and said dimensions of said physical profile are determined to be corresponding dimensions of said one of said profile shapes.

20 26. The method of claim 25 wherein said optical path includes a focusing mechanism.

27. The method of claim 25 wherein said measuring of said diffracted light involves a measurement of intensity of said diffracted light.

28. The method of claim 25 wherein said measuring of said diffracted light involves a measurement of intensity of said diffracted light, and a phase difference between polarizations of said diffracted light.

29. The method of claim 28 wherein said comparing of said measured diffraction spectrum with said calculated diffraction spectra in said library to determine a best-match calculated spectrum is performed using a least squares computation.

5       30. A method for analyzing the profile of a workpiece comprising:  
generating intra-layer-dependent portions of diffraction calculations for a plurality of profile shapes;  
caching said intra-layer-dependent portions of said diffraction calculations in a memory;

10       generating calculated-diffraction spectra for said profile shapes based on said intra-layer-dependent portions of said diffraction calculations retrieved from said memory;  
generating a library of said profile shapes and said calculated-diffraction spectra;  
illuminating a portion of the workpiece with incident radiation;  
15       measuring radiation diffracted from said portion of the workpiece;  
obtaining a measured-diffraction spectrum based on the measurement of the diffraction radiation;  
matching said measured-diffraction spectrum with one of said plurality of calculated-diffraction spectra contained in said library; and  
20       selecting the profile shape associated with the calculated-diffraction spectrum that matches said measured-diffraction spectrum.

31. The method of claim 30 further comprising intra-layer parameters associated with said profile shapes and incident-radiation parameters associated with said incident

radiation, and wherein said step of generating intra-layer-dependent portions further comprises:

determining an intra-layer range and an intra-layer increment of said intra-layer parameters;

5 determining an incident-radiation range and an incident-radiation increment of said incident-radiation parameters; and

generating said intra-layer-dependent portions of said diffraction calculations for said intra-layer parameters between said intra-layer range at said intra-layer increment, and for said incident-radiation parameters between said incident-radiation range at said 10 incident-radiation increment.

32. The method of claim 30 wherein said measuring step further comprises measuring the intensity of said diffracted radiation.

33. The method of claim 32 further comprising the step of measuring a phase difference between said incident radiation and said diffracted radiation.

15 34. The method of claim 30 wherein said matching step is performed utilizing a least square computation.

35. The method of claim 34 further comprising:

selecting a plurality of sample wavelengths;

obtaining a difference at each sample wavelength by subtracting said measured-

20 diffraction spectrum with said calculated-diffraction spectrum at said sample wavelength; and

squaring said difference; and

summing said difference.

36. The method of claim 30 wherein said illuminating step further comprises focusing said incident radiation.

37. The method of claim 36 wherein said incident radiation includes light having a plurality of wavelengths, and wherein the portion of the workpiece is illuminated from 5 a single angle.

38. The method of claim 30 wherein said incident radiation includes light having a single wavelength, and wherein the portion of the workpiece is illuminated from a plurality of angles.

39. A method of analyzing the metrology of a semi-conductor wafer utilizing an 10 incident light having a plurality of wavelengths, said method comprising:

providing a library of a plurality of profile shapes and a plurality of calculated-diffraction spectra, wherein each profile shape is associated with each calculated-diffraction spectrum;

focusing the incident light;

15 illuminating a portion of the wafer from a single incident angle;

measuring light diffracted from said portion of the wafer;

obtaining a measured-diffraction spectrum based on the measurement of the diffracted light;

comparing said measured-diffraction spectrum with said calculated-diffraction 20 spectrum; and

obtaining a profile for the wafer based on said comparison.

40. The method of claim 39 wherein said generating step further comprises:

1000 900 800 700 600 500 400 300 200 100 0

determining an intra-layer range and an intra-layer increment of intra-layer parameters associated with said profile shapes;

determining an incident-light range and an incident-light increment of incident-light parameters associated with said incident light;

5 generating intra-layer-dependent portions of diffraction calculations for said intra-layer parameters between said intra-layer range at said intra-layer increment, and for said incident-light parameters between said incident-light range at said incident-light increment; and

10 generating said calculated-diffraction spectra based on said intra-layer dependent portions.

41. The method of claim 39 wherein said comparing step further comprises:

selecting a plurality of sample wavelengths;

obtaining a difference at each sample wavelength by subtracting said measured-diffraction spectrum with said calculated-diffraction spectrum at said sample wavelength;

15 and

squaring said difference; and

summing said difference.

42. The method of claim 39 wherein said measuring step further comprises:

measuring the intensity of the diffracted light; and

20 measuring a phase difference between said incident light and said diffracted light.

43. A method of analyzing the profile of a workpiece utilizing an incident light having a single wavelength, said method comprising:

generating a library of profile shapes;

determining an intra-layer range and an intra-layer increment of intra-layer parameters associated with said profile shapes;

determining an incident-light range and an incident-light increment of incident-light parameters associated with said incident light;

5 generating intra-layer-dependent portions of diffraction calculations for said intra-layer parameters between said intra-layer range at said intra-layer increment, and for said incident-light parameters between said incident-light range at said incident-light increment;

generating a plurality of calculated-diffraction spectrum based on said intra-layer dependent portions;

10 storing said plurality of calculated-diffraction spectrum in said library of profile shapes, wherein each calculated-diffraction spectrum is associated with each profile shape;

illuminating a portion of the wafer from a plurality of incident angles;

15 measuring light diffracted from said portion of the wafer;

obtaining a measured-diffraction spectrum based on the measurement of the diffracted light;

comparing said measured-diffraction spectrum with said calculated-diffraction spectrum; and

20 obtaining a profile for the wafer based on said comparison.

44. The method of claim 43 further comprising:

caching said pre-calculated intra-layer-dependent portions of said diffraction calculations.

45. A method of analyzing the profile of a workpiece utilizing an incident light, wherein the workpiece has a plurality of layers, said method comprising:

- generating a library of profile shapes;
- determining an intra-layer range and an intra-layer increment of intra-layer
- 5 parameters associated with said profile shapes;
- determining an incident-light range and an incident-light increment of incident-light parameters associated with said incident light;
- generating intra-layer-dependent portions of diffraction calculations for said intra-layer parameters between said intra-layer range at said intra-layer increment, and for said
- 10 incident-light parameters between said incident-light range at said incident-light increment;
- generating a plurality of calculated-diffraction spectrum based on said intra-layer dependent portions;
- storing said plurality of calculated-diffraction spectrum in said library of profile
- 15 shapes, wherein each calculated-diffraction spectrum is associated with each profile shape;
- illuminating a portion of the workpiece with said incident light;
- measuring light diffracted from said portion of the workpiece;
- obtaining a measured-diffraction spectrum based on the measurement of the
- 20 diffracted light;
- comparing said measured-diffraction spectrum with said calculated-diffraction spectrum; and
- obtaining a profile for the layers of the workpiece based on said comparison.

46. The method of claim 45 wherein said comparing step further comprises:  
selecting a plurality of sample wavelengths;  
obtaining a difference at each sample wavelength by subtracting said measured-diffraction spectrum with said calculated-diffraction spectrum at said sample wavelength;  
5 and  
squaring said difference; and  
summing said difference.

47. The method of claim 45 wherein said measuring step further comprises:  
measuring the intensity of the diffracted light; and  
measuring a phase difference between said incident light and said diffracted light.

48. A system for analyzing the profile of a workpiece comprising:  
an electromagnetic radiation source configured to illuminate a portion of the workpiece with an incident radiation;  
a photometer configured to measure radiation diffracted from the workpiece;  
15 a library having a plurality of profile shapes and a plurality of calculated-diffraction spectra, wherein said calculated-diffraction spectra were generated based on intra-layer dependent portions of diffraction calculations of said profile shapes; and  
a processor configured to compare said measured-diffraction spectrum with said calculated-diffraction spectrum to obtain a profile of the workpiece.

20 49. The system of claim 48 further comprising a cache of said intra-layer dependent portions of diffraction calculations, wherein said intra-layer dependent portions were generated for intra-layer parameters associated with said profile shapes, between an intra-layer range at an intra-layer increment and for incident-light parameters

associated with said incident light, between an incident-light range at an incident-light increment.

50. The system of claim 48 further comprising a focus lens configured to focus said incident radiation.

5 51. The system of claim 48 wherein said incident radiation includes light having a plurality of wavelengths.

52. The system of claim 48 wherein said incident radiation includes light having a single wavelength.

53. The system of claim 48 wherein said photometer is configured to measure the 10 intensity of said diffracted radiation.

54. The system of claim 53 wherein said photometer is configured to measure a phase difference between said incident radiation and said diffracted radiation.

55. The system of claim 48 wherein said processor is further configured to 15 perform a least square computation.

56. A system for analyzing the profile of a workpiece utilizing an incident light, wherein the workpiece has a plurality of layers, said system comprising:

means for generating a library of profile shapes;

means for determining an intra-layer range and an intra-layer increment of intra-layer parameters associated with said profile shapes;

20 means for determining an incident-light range and an incident-light increment of incident-light parameters associated with said incident light;

means for generating intra-layer-dependent portions of diffraction calculations for said intra-layer parameters between said intra-layer range at said intra-layer increment,

and for said incident-light parameters between said incident-light range at said incident-light increment;

means for generating a plurality of calculated-diffraction spectrum based on said intra-layer dependent portions;

5 means for storing said plurality of calculated-diffraction spectrum in said library of profile shapes, wherein each calculated-diffraction spectrum is associated with each profile shape;

means for illuminating a portion of the workpiece with said incident light;

means for measuring light diffracted from said portion of the workpiece;

0 means for obtaining a measured-diffraction spectrum based on the measurement of the diffracted light;

means for comparing said measured-diffraction spectrum with said calculated-diffraction spectrum; and

15 means for obtaining a profile for the layers of the workpiece based on said comparison.